=> d his

(FILE 'HOME' ENTERED AT 15:06:30 ON 25 FEB 2000)

FILE 'HCAPLUS' ENTERED AT 15:06:37 ON 25 FEB 2000
L1 823 S COOK P?/AU
L2 46 S L1 AND COMBINAT?
L3 6 S L2 AND HETEROCYC?
SELECT RN L3 1-6

FILE 'REGISTRY' ENTERED AT 15:07:03 ON 25 FEB 2000
L4 200 S E1-200
L5 278 S E200-477
L6 477 S L4 OR L5
L7 25 S L6 AND NCNC3/ES
L8 28 S L6 AND NCNC2-NCNC3/ES
L9 53 S L7 OR L8

FILE 'HCAPLUS' ENTERED AT 15:08:58 ON 25 FEB 2000
L10 4 S L3 AND L9
L11 2 S L3 NOT L10

=> d all

L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:379847 HCAPLUS
DN 131:170275
TI A solution-phase **combinatorial** chemistry methodology for drug discovery
AU An, Haoyun; **Cook, P. Dan**
CS Isis Pharmaceuticals, Inc, Carlsbad, CA, 92008, USA
SO Recent Res. Dev. Org. Chem. (1998), 2(Pt. 2), 473-488
CODEN: RDOCFJ
PB Transworld Research Network
DT Journal; General Review
LA English
CC 28-0 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
AB In this review with 22 refs., recent work on soln.-phase simultaneous addn. of functionalities (SPSAF) done by the Isis Pharmaceutical group is discussed. The details of the SPSAF **combinatorial** synthesis of libraries from a variety of novel, unsym. linear, polyazamacrocyclic, and **heterocyclic** scaffolds is described. Diverse, complex libraries generated by the SPSAF approach, library purifn. and confirmation techniques, and the biol. evaluation of resulting libraries for antibacterial and RNA interaction assays are summarized.
ST review soln phase **combinatorial** chem drug discovery
IT Antibacterial agents
Combinatorial chemistry
Drug design
(review of soln.-phase **combinatorial** chem. methodol. for drug discovery)
IT Macrocyclic nitrogen **heterocycles**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(review of soln.-phase **combinatorial** chem. methodol. for drug discovery)

=> d all 2

L11 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:112234 HCAPLUS
DN 128:167445
TI Preparation of dinitrogen **heterocycle** compounds as antibacterial agents
IN **Cook, Phillip Dan**; Kawasaki, Andrew M.; Kung, Pei Pei
PA Isis Pharmaceuticals, Inc., USA; Cook, Phillip Dan; Kawasaki, Andrew M.; Kung, Pei Pei
SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-495
ICS C07D241-04
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 10
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9805332	A1	19980212	WO 1997-US13686	19970801
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, US, US, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5731438	A	19980324	US 1996-691185	19960801
	US 5798360	A	19980825	US 1996-688993	19960801
	US 5817489	A	19981006	US 1996-691149	19960801
	US 5922872	A	19990713	US 1996-691139	19960801
	AU 9739069	A1	19980225	AU 1997-39069	19970801
	US 5998419	A	19991207	US 1998-40787	19980318

PRAI US 1996-688993 19960801
US 1996-691139 19960801
US 1996-691149 19960801
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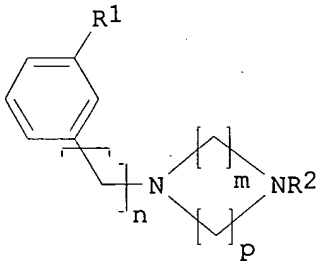
WO 1997-US13686 19970801
OS MARPAT 128:167445
GI



I

Searched by John Dantzman 308-4488

AB Dinitrogen **heterocycle** compds. I [n, m, p = 1, 2, 3; R1 = halo, cyano, alkyl, perhaloalkyl, alkoxy, NO2, NO, carboxylate; R2 = H, alkyl, aryl, alkaryl, **heterocyclyl**, etc.], contg. at least one N-meta-substituted alkaryl group and/or novel meta-benzylic compds., were prepd. E.g., a soln. of tert-Bu 1-piperazinecarboxylate was treated with a mixt. of benzyl bromide, 3-methylbenzyl bromide, 3-trifluoromethylbenzyl bromide, 3-fluorobenzyl bromide, 3-(methoxycarbonyl)benzyl bromide, 3-cyanobenzyl bromide, and 3-nitrobenzyl bromide to give a mixt. of tert-Bu 4-(substituted benzyl)-1-piperazinecarboxylates. The antibacterial activity of I toward staphylococcus aureus and E. coli imp- was detd.

ST dinitrogen **heterocycle combinatorial** library prepn; piperazine deriv **combinatorial** library prepn; antibacterial agent dinitrogen **heterocycle combinatorial** library

IT Antibacterial agents
Combinatorial library
(prepn. of **combinatorial** libraries of dinitrogen **heterocycles** as antibacterial agents)

IT 203047-40-9P 203047-41-0P 203047-42-1P 203047-43-2P 203047-44-3P
203047-45-4P 203047-46-5P 203047-47-6P 203047-48-7P 203047-49-8P
203047-50-1P 203047-51-2P 203047-52-3P 203047-53-4P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of **combinatorial** libraries of dinitrogen **heterocycles** as antibacterial agents)

IT 203048-28-6P 203048-29-7P 203048-30-0P 203048-31-1P 203048-32-2P
203048-33-3P 203048-34-4P 203048-35-5P 203048-36-6P 203048-37-7P
203048-38-8P 203048-39-9P 203048-40-2P 203048-41-3P 203048-42-4P
203048-43-5P 203048-44-6P 203048-45-7P 203048-46-8P 203048-47-9P
203048-48-0P 203048-49-1P 203048-50-4P 203048-51-5P 203048-52-6P
203048-53-7P 203048-54-8P 203048-55-9P 203048-56-0P 203048-57-1P
203048-58-2P 203048-59-3P 203048-60-6P 203048-61-7P 203048-62-8P
203048-63-9P 203048-64-0P 203048-65-1P 203048-66-2P 203048-67-3P
203048-68-4P 203048-69-5P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of **combinatorial** libraries of dinitrogen **heterocycles** as antibacterial agents)

IT 92-54-6, N-Phenylpiperazine 100-39-0, Benzyl bromide 104-94-9, 4-Methoxyaniline 110-85-0, Piperazine, reactions 136-95-8, 2-Aminobenzothiazole 402-23-3, 3-Trifluoromethylbenzyl bromide 456-41-7, 3-Fluorobenzyl bromide 620-13-3, 3-Methylbenzyl bromide 1129-28-8 2687-43-6, O-Benzylhydroxylamine hydrochloride 3958-57-4, 3-Nitrobenzyl bromide 5452-35-7, Cycloheptylamine 15532-75-9 28188-41-2, 3-Cyanobenzyl bromide 41202-32-8 57260-71-6, tert-Butyl 1-piperazinecarboxylate 67442-07-3 127561-18-6 175334-69-7
RL: RCT (Reactant)
(prepn. of **combinatorial** libraries of dinitrogen **heterocycles** as antibacterial agents)

IT 2759-28-6P 5321-48-2P 29182-87-4P 55513-16-1P 55513-19-4P
57260-70-5P 77278-55-8P 78158-32-4P 121189-77-3P 191598-96-6P

203047-32-9P 203047-33-0P 203047-34-1P 203047-35-2P 203047-36-3P
203047-37-4P 203047-38-5P 203047-39-6P 203047-54-5P 203047-55-6P
203047-56-7P 203047-57-8P 203047-58-9P 203047-59-0P 203047-60-3P
203047-88-5P 203047-89-6P 203047-90-9P 203047-91-0P 203047-92-1P
203047-93-2P 203047-94-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of **combinatorial** libraries of dinitrogen **heterocycles** as antibacterial agents)

IT 3074-46-2P 36824-73-4P 94012-33-6P 203047-61-4P 203047-62-5P
203047-63-6P 203047-64-7P 203047-65-8P 203047-66-9P 203047-67-0P
203047-68-1P 203047-69-2P 203047-70-5P 203047-71-6P 203047-72-7P
203047-73-8P 203047-74-9P 203047-75-0P 203047-76-1P 203047-77-2P
203047-78-3P 203047-79-4P 203047-80-7P 203047-81-8P 203047-82-9P
203047-83-0P 203047-84-1P 203047-85-2P 203047-86-3P 203047-87-4P
203047-95-4P 203047-96-5P 203047-97-6P 203047-98-7P 203047-99-8P
203048-00-4P 203048-01-5P 203048-02-6P 203048-03-7P 203048-04-8P
203048-05-9P 203048-06-0P 203048-07-1P 203048-08-2P 203048-09-3P
203048-10-6P 203048-11-7P 203048-12-8P 203048-13-9P 203048-14-0P
203048-15-1P 203048-16-2P 203048-17-3P 203048-18-4P 203048-19-5P
203048-20-8P 203048-21-9P 203048-22-0P 203048-23-1P 203048-24-2P
203048-25-3P 203048-26-4P 203048-27-5P 203048-70-8P 203048-71-9P
203048-72-0P 203048-73-1P 203048-74-2P 203048-75-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of **combinatorial** libraries of dinitrogen **heterocycles** as antibacterial agents)

=> d bib abs hitstr l10

L10 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:42619 HCAPLUS
DN 130:110283
TI Nucleobase **heterocyclic combinatorialization**
IN **Cook, Phillip Dan**; An, Haoyun; Guinosso, Charles J.; Fraser, Allister S.; Kawasaki, Andrew M.
PA Isis Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9900669	A1	19990107	WO 1998-US13666	19980630
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9881791	A1	19990119	AU 1998-81791	19980630

PRAI US 1997-884873 19970630
WO 1998-US13666 19980630
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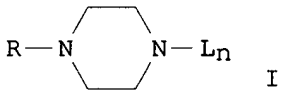
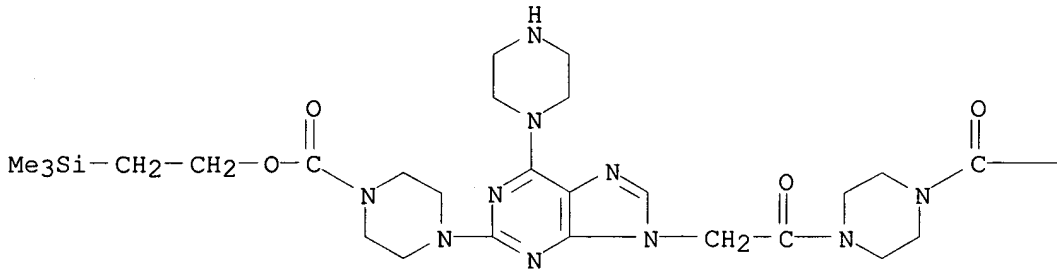


I

AB Mixts. of title compds. [I; Ln = alkyl, alkynyl, carbocycloalkyl, aryl, heteroaryl, etc.; R = C6H5, 2-pyrimidyl, 2-purinyl, etc.] are prepd., preferably in soln. phase from the reaction of a purine or pyrimidine **heterocyclic** scaffold with a set of related chem. substituents, optionally through employment of a tether moiety, having antibacterial and other biol. activities per se and are articles of commerce. Thus, the title compd. I (Ln = 2-(4-BOC-1-piperazinyl-6-aminopyrimidyl); R = BOC) was prepd. from 2,4,6-trichloropyrimidine and I (R = H; Ln = BOC).
IT **219688-02-5P 219688-03-6P 219688-47-8P**
219688-51-4P 219688-61-6P 219688-66-1P
219688-72-9P 219688-84-3P 219688-88-7P
219688-92-3P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant);
SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(**combinatorialization** of nucleobase **heterocyclic**)
RN 219688-02-5 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[9-[2-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-oxoethyl]-6-(1-piperazinyl)-9H-purin-2-yl]-, 2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

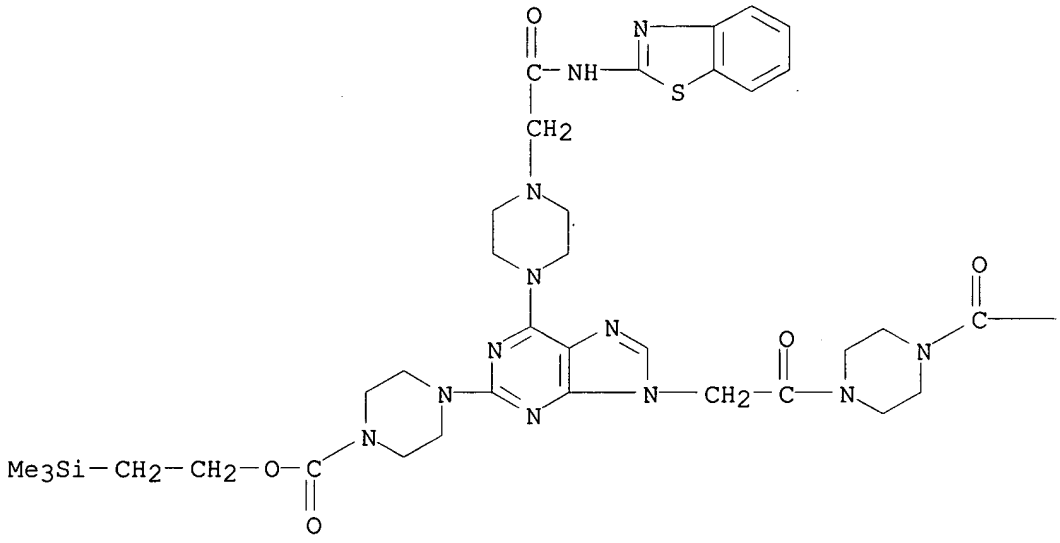


PAGE 1-B

—OBu-t

RN 219688-03-6 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-9-[2-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-oxoethyl]-9H-purin-2-yl]-, 2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)

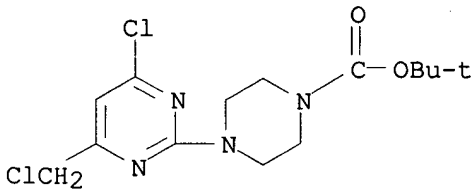
PAGE 1-A



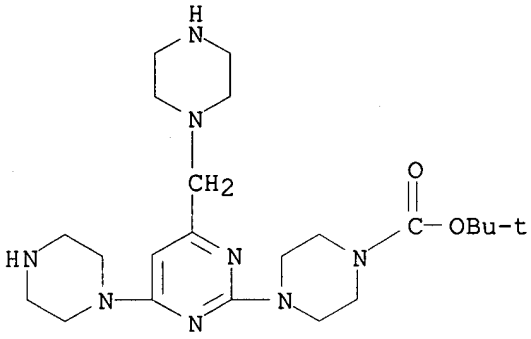
PAGE 1-B

— OBu-t

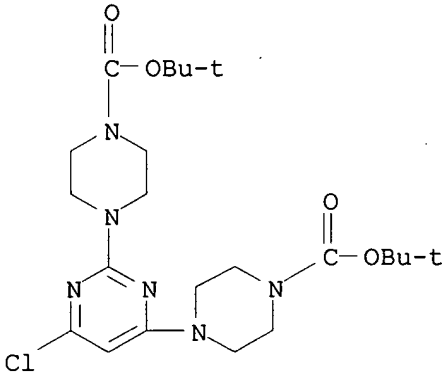
RN 219688-47-8 HCAPLUS
CN 1-Piperazinecarboxylic acid,
4-[4-chloro-6-(chloromethyl)-2-pyrimidinyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



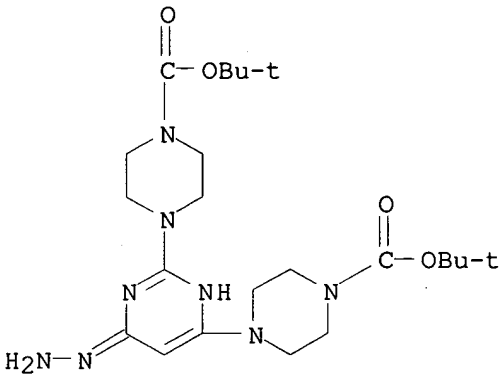
RN 219688-51-4 HCAPLUS
CN 1-Piperazinecarboxylic acid,
4-[4-(1-piperazinyl)-6-(1-piperazinylmethyl)-
2-pyrimidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



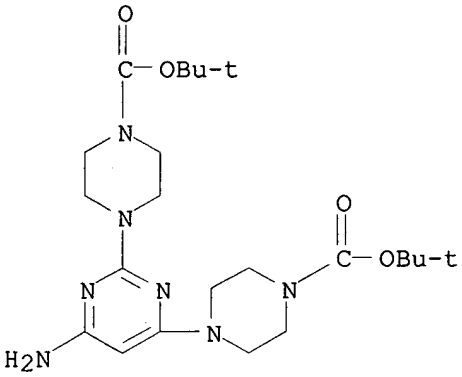
RN 219688-61-6 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-(6-chloro-2,4-pyrimidinediyl)bis-,
bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 219688-66-1 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-(6-hydrazino-2,4-pyrimidinediyl)bis-,
bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 219688-72-9 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-(6-amino-2,4-pyrimidinediyl)bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



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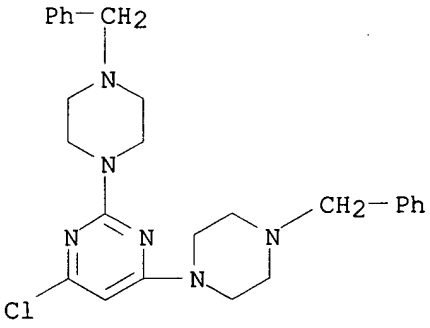
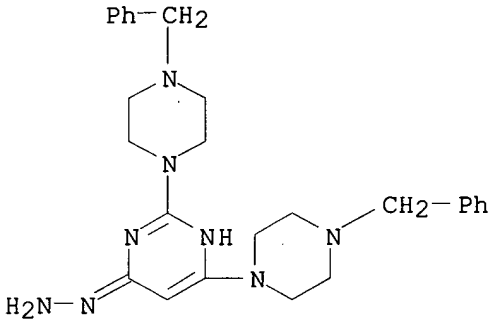
CN Pyrimidine, 4-chloro-2,6-bis[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

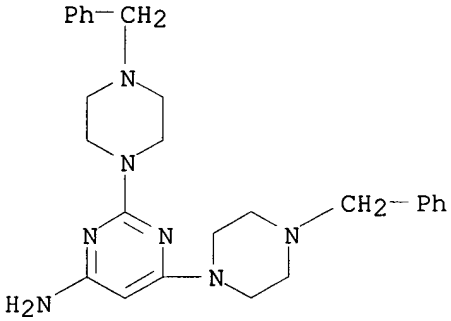


Searched by John Dantzman 308-4488

RN 219688-88-7 HCAPLUS
CN 4(1H)-Pyrimidinone, 2,6-bis[4-(phenylmethyl)-1-piperazinyl]-, hydrazone (9CI) (CA INDEX NAME)



RN 219688-92-3 HCAPLUS
CN 4-Pyrimidinamine, 2,6-bis[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



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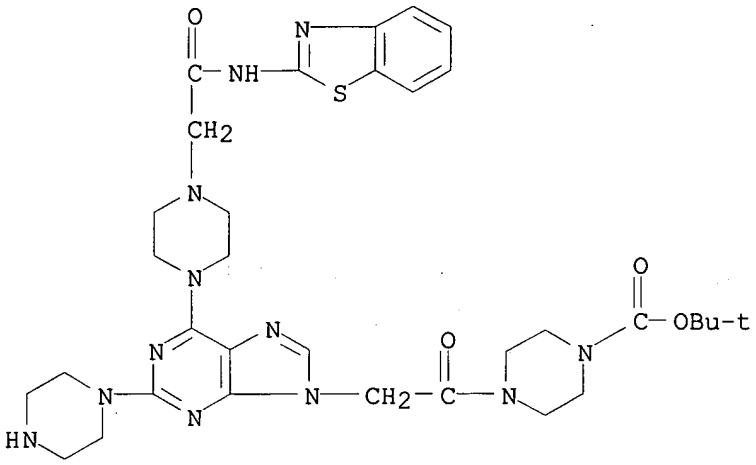
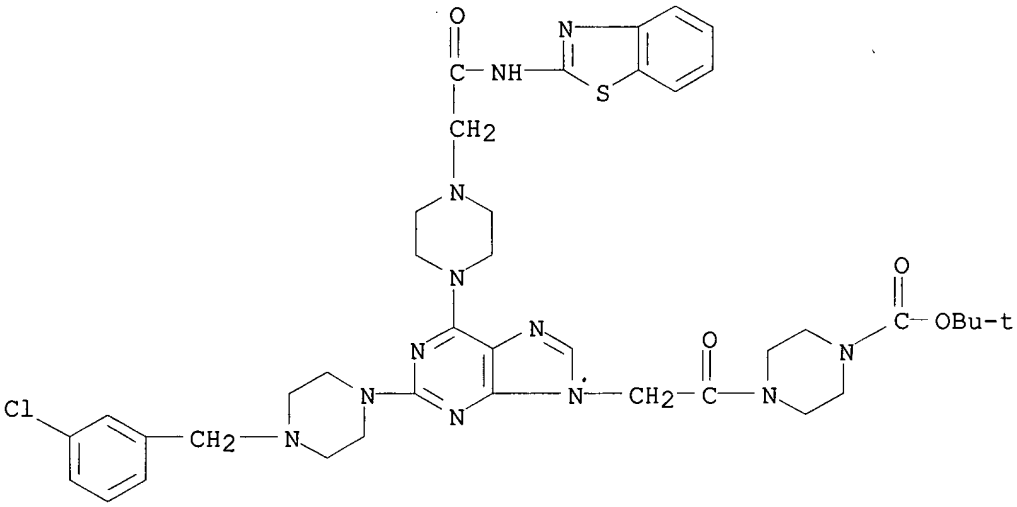
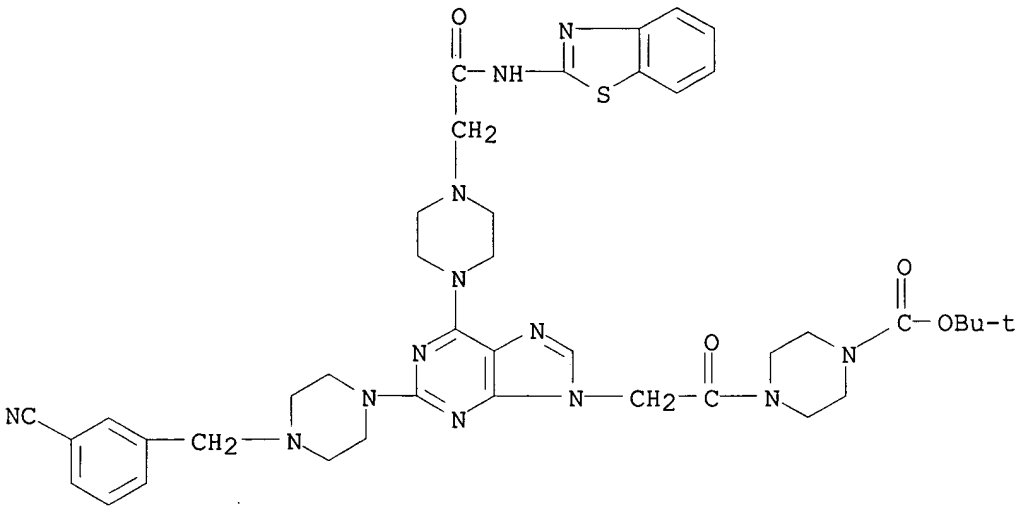
219688-10-5P 219688-11-6P 219688-12-7P
219688-13-8P 219688-14-9P 219688-56-9P
219688-78-5P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(**combinatorialization** of nucleobase **heterocyclic**)
RN 219688-04-7 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-(1-piperazinyl)-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 219688-05-8 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[(3-chlorophenyl)methyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 219688-06-9 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[(3-cyanophenyl)methyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 219688-07-0 HCAPLUS
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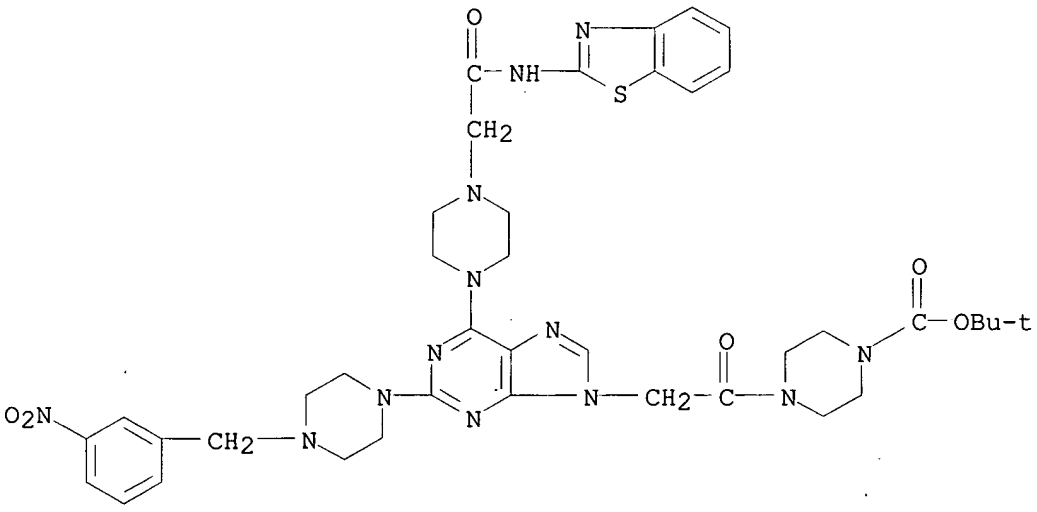
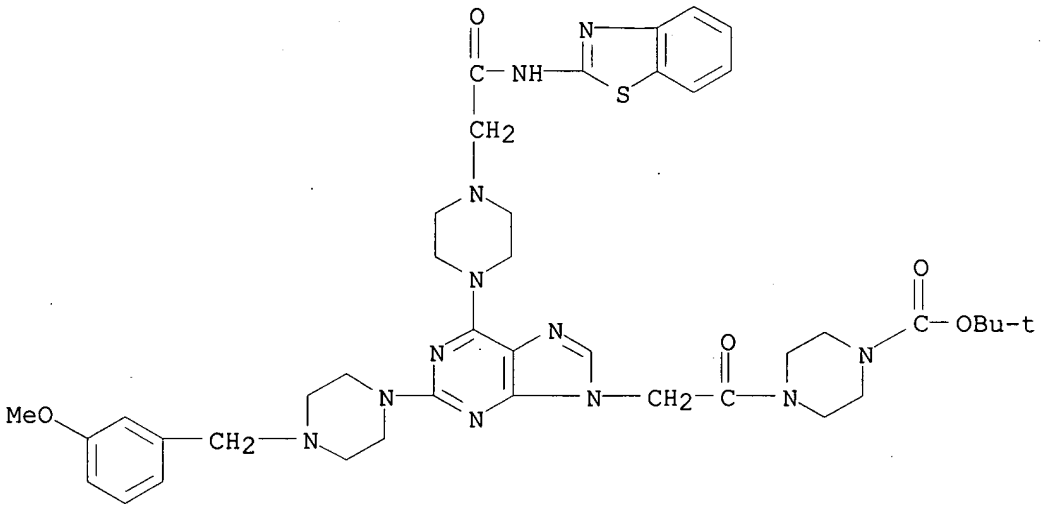
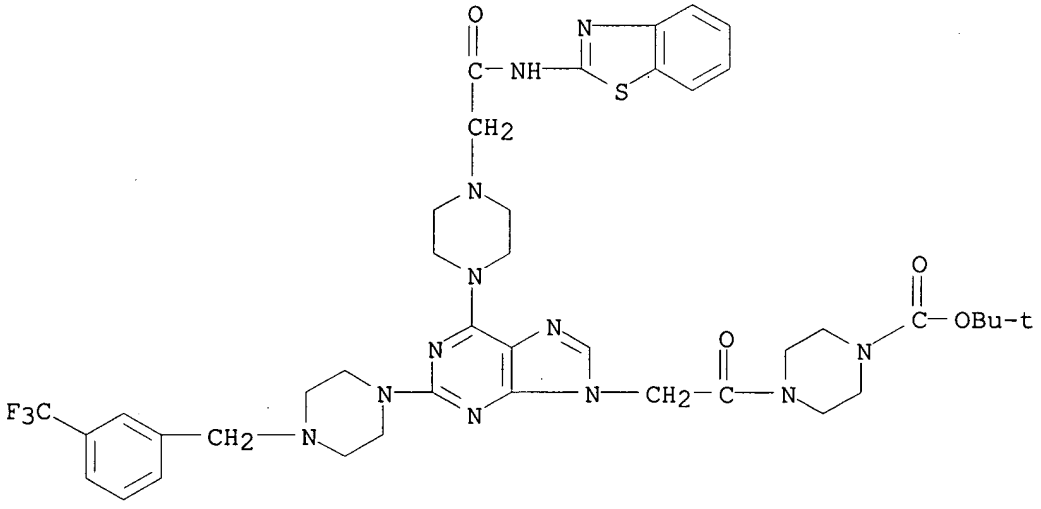


RN 219688-08-1 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[(3-methoxyphenyl)methyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

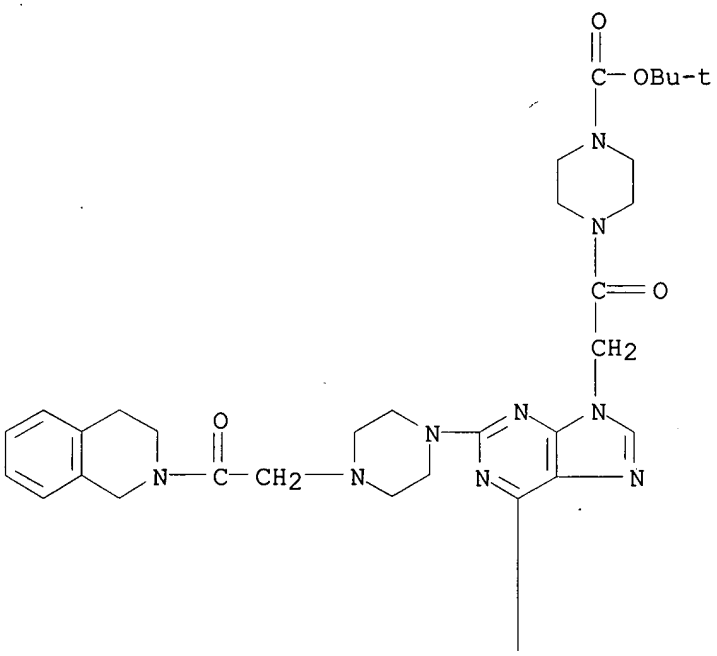


RN 219688-09-2 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[[3-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

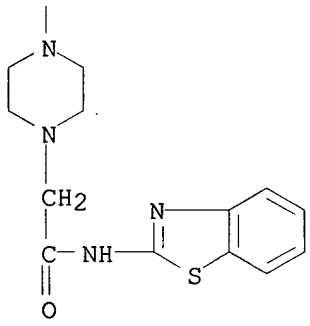


RN 219688-10-5 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[2-(3,4-dihydro-2(1H)-isoquinolinyl)-2-oxoethyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

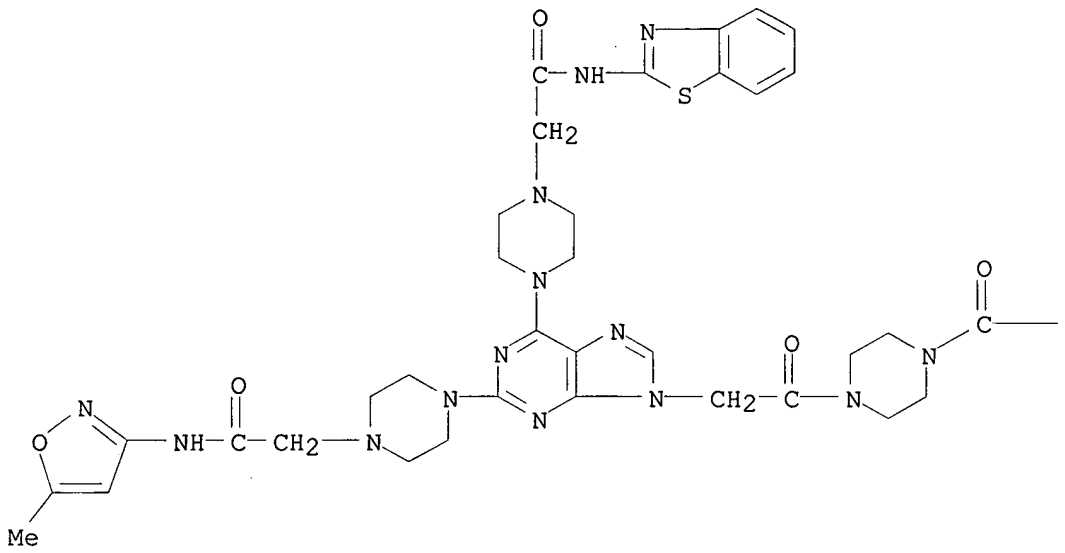


PAGE 2-A



RN 219688-11-6 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[2-[(5-methyl-3-isoxazolyl)amino]-2-oxoethyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

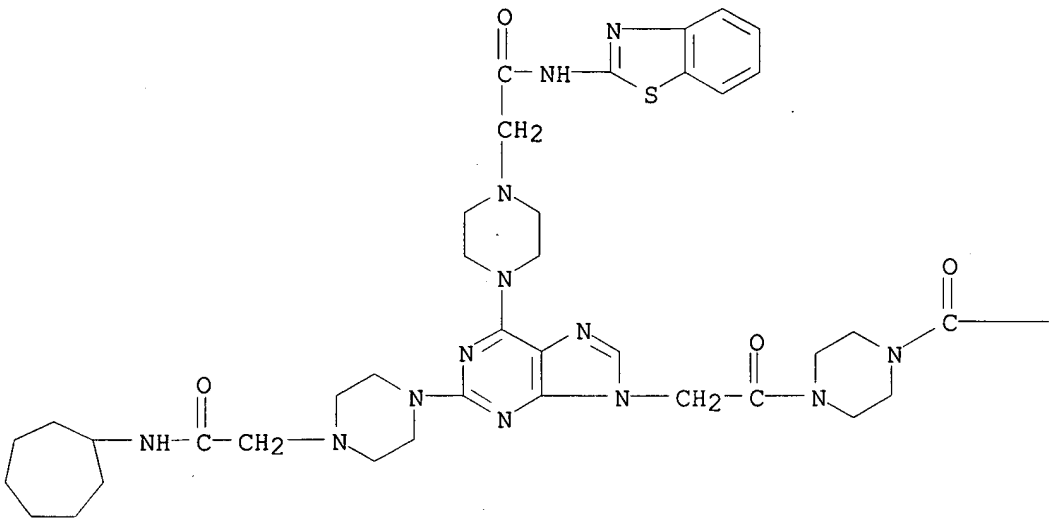


PAGE 1-B

— OBu-t

RN 219688-12-7 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[6-[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-2-[4-[2-(cycloheptylamino)-2-oxoethyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

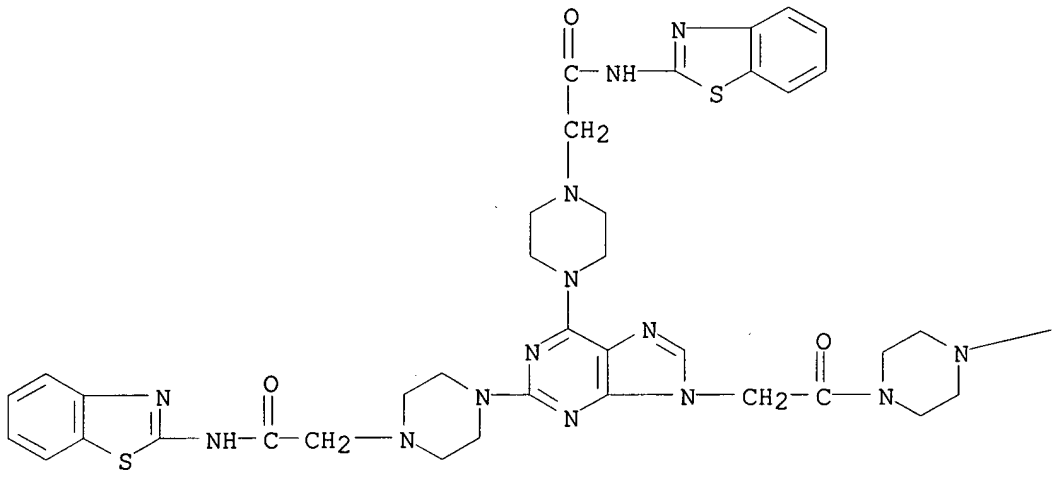


PAGE 1-B

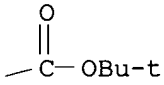
—OBu-t

RN 219688-13-8 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[2,6-bis[4-[2-(2-benzothiazolylamino)-2-oxoethyl]-1-piperazinyl]-9H-purin-9-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

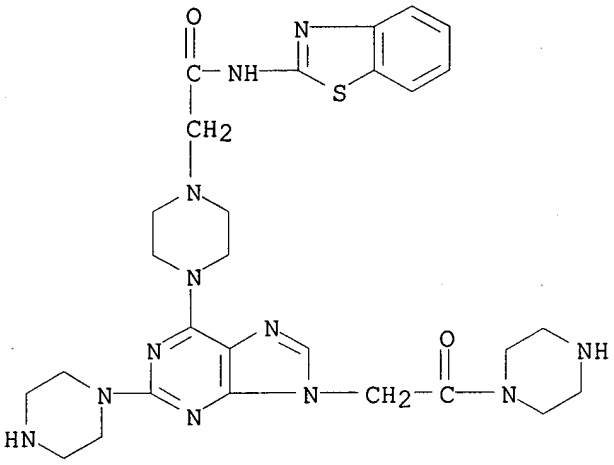
PAGE 1-A



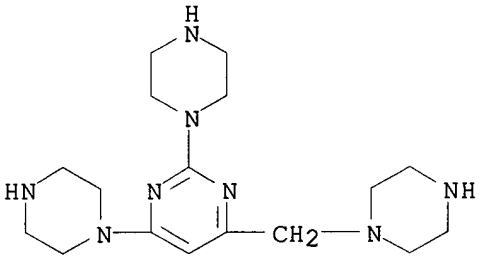
PAGE 1-B



RN 219688-14-9 HCAPLUS
CN 1-Piperazineacetamide, N-2-benzothiazolyl-4-[9-[2-oxo-2-(1-piperazinyl)ethyl]-2-(1-piperazinyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

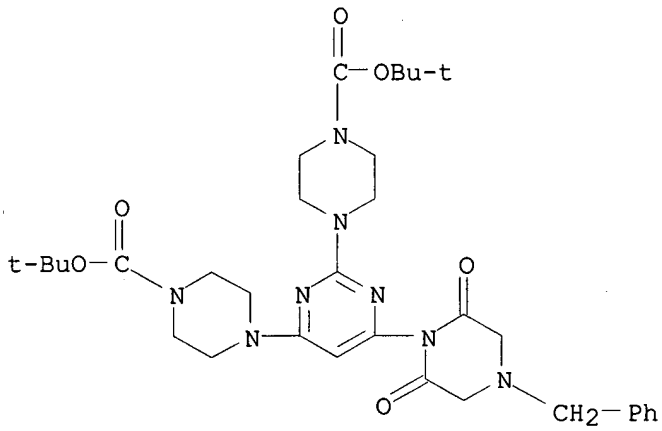


RN 219688-56-9 HCAPLUS
CN Pyrimidine, 2,4-di-1-piperazinyl-6-(1-piperazinylmethyl)-, hexahydrochloride (9CI) (CA INDEX NAME)

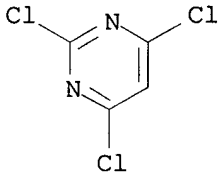


● 6 HCl

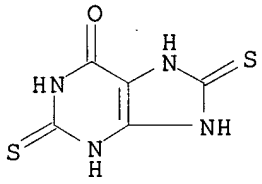
RN 219688-78-5 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-[6-[2,6-dioxo-4-(phenylmethyl)-1-piperazinyl]-2,4-pyrimidinediyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



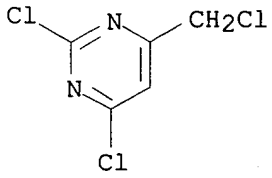
IT **3764-01-0**, 2,4,6-Trichloropyrimidine **15986-32-0**
94170-66-8
RL: RCT (Reactant)
(**combinatorialization** of nucleobase **heterocyclic**)
RN 3764-01-0 HCAPLUS
CN Pyrimidine, 2,4,6-trichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



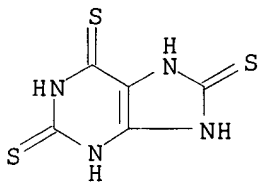
RN 15986-32-0 HCAPLUS
CN 6H-Purin-6-one, 1,2,3,7,8,9-hexahydro-2,8-dithioxo- (9CI) (CA INDEX NAME)



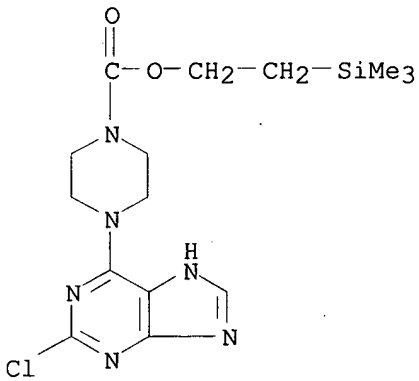
RN 94170-66-8 HCAPLUS
CN Pyrimidine, 2,4-dichloro-6-(chloromethyl)- (9CI) (CA INDEX NAME)



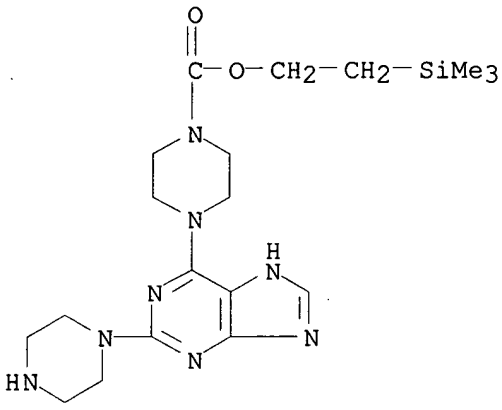
IT **15986-33-1P**, 2,6,8-Trimercaptopurine **219687-94-2P**
219687-95-3P 219687-96-4P 219687-97-5P
219687-98-6P 219687-99-7P 219688-00-3P
219689-21-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(**combinatorialization** of nucleobase **heterocyclic**)
RN 15986-33-1 HCAPLUS
CN 1H-Purine-2,6,8(3H)-trithione, 7,9-dihydro- (9CI) (CA INDEX NAME)



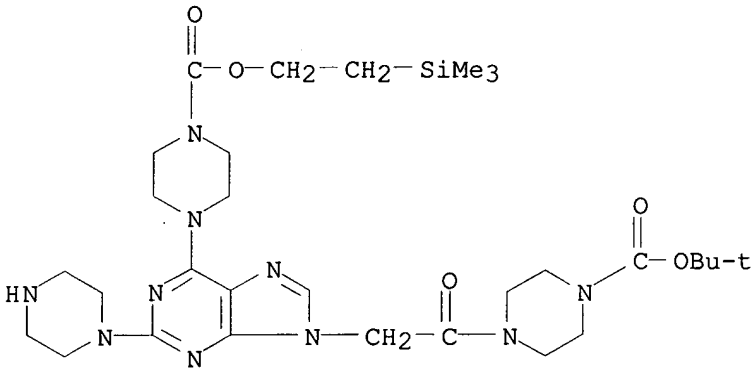
RN 219687-94-2 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-(2-chloro-1H-purin-6-yl)-,
2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)



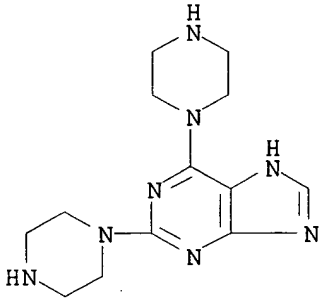
RN 219687-95-3 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-(1-piperazinyl)-1H-purin-6-yl]-,
2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)



RN 219687-96-4 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[9-[2-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-oxoethyl]-2-(1-piperazinyl)-9H-purin-6-yl]-, 2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)



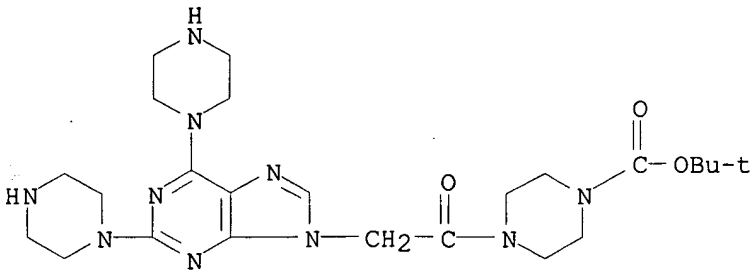
RN 219687-97-5 HCAPLUS
CN 1H-Purine, 2,6-di-1-piperazinyl- (9CI) (CA INDEX NAME)



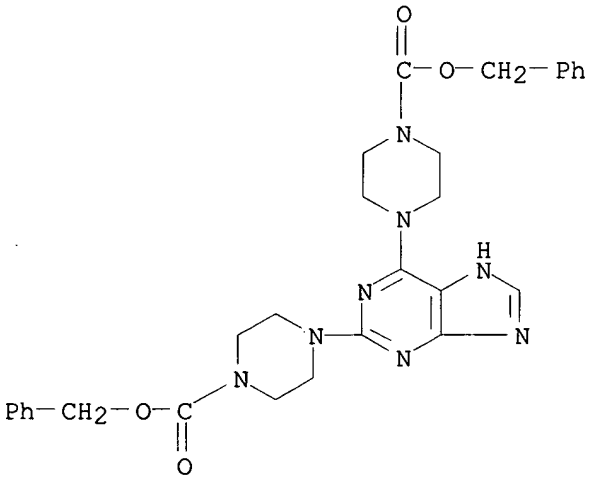
RN 219687-98-6 HCAPLUS

Searched by John Dantzman 308-4488

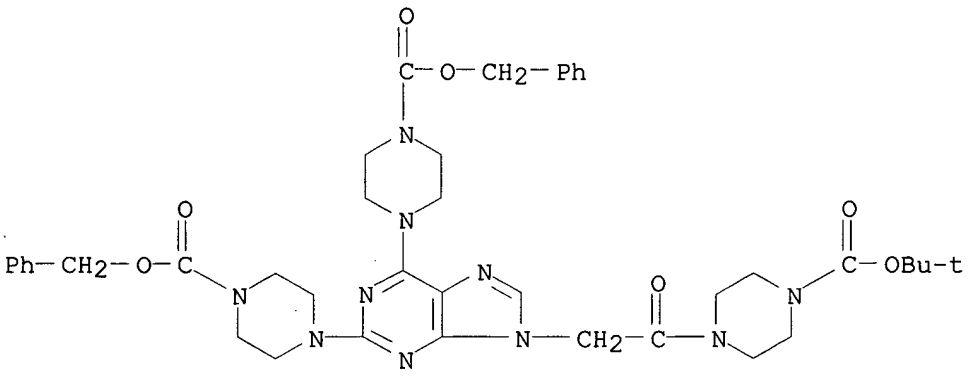
CN 1-Piperazinecarboxylic acid, 4-[(2,6-di-1-piperazinyl-9H-purin-9-yl)acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



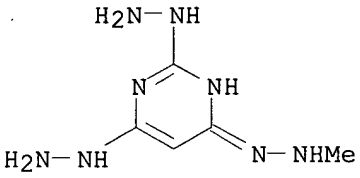
RN 219687-99-7 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-(1H-purine-2,6-diyl)bis-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



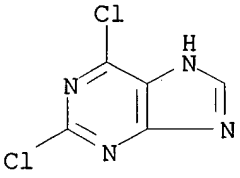
RN 219688-00-3 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-[9-[2-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-oxoethyl]-9H-purine-2,6-diyl]bis-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



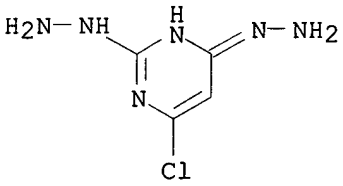
RN 219689-21-1 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 6-hydrazino-, 2-hydrazone 4-(methylhydrazone) (9CI) (CA INDEX NAME)



IT **5451-40-1**, 2,6-Dichloropurine
RL: RCT (Reactant)
(**combinatorialization** of nucleobase **heterocyclic** piperazines)
RN 5451-40-1 HCAPLUS
CN 1H-Purine, 2,6-dichloro- (9CI) (CA INDEX NAME)



IT **6972-15-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(**combinatorialization** of nucleobase **heterocyclic** piperazines)
RN 6972-15-2 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 6-chloro-, dihydrazone (9CI) (CA INDEX NAME)



=> d bib abs hitstr l10 2

L10 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:118624 HCAPLUS
DN 128:167656
TI **Combinatorial** library on the preparation of oligodeoxyribonucleotide phosphoramidates and phosphorothiomidates as phospholipase A2 inhibitors
IN **Cook, Phillip Dan**; Acevedo, Oscar; Hebert, Normand
PA ISIS Pharmaceuticals, Inc., USA
SO U.S., 26 pp. Cont.-in-part of U.S. 5,637,684.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5717083	A	19980210	US 1996-693112	19960819
US 5637684	A	19970610	US 1994-200638	19940223
WO 9523160	A1	19950831	WO 1995-US2267	19950223

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

PRAI US 1994-200638 19940223
WO 1995-US2267 19950223
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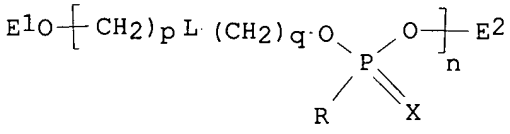
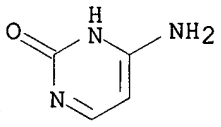
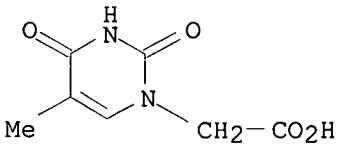


I

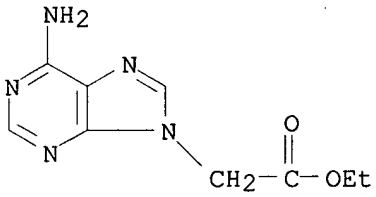
AB **Combinatorial** library on the prepn. of title oligodeoxyribonucleotides I (X = O, S; R = amine, N-contg. **heterocycle**; L = alkyl, alkenyl, alkynyl, carbocycle, **heterocycle**; E1, E2 = independently H, hydroxyl protecting group, activated solid support; p, q = 0-6; n = 2-50) were prepd. as phospholipase A2 inhibitors.
IT **71-30-7**, Cytosine
RL: RCT (Reactant)
(**combinatorial** library on the prepn. of oligodeoxyribonucleotide phosphoramidates and phosphorothiomidates as phospholipase A2 inhibitors)
RN 71-30-7 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino- (9CI) (CA INDEX NAME)



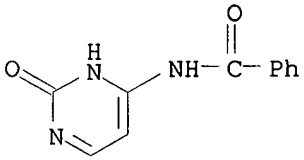
IT **20924-05-4P 25477-96-7P 26661-13-2P,**
N-Benzoylcytosine **168263-86-3P 171406-46-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(**combinatorial** library on the prepn. of oligodeoxyribonucleotide phosphoramidates and phosphorothiomidates as phospholipase A2 inhibitors)
RN 20924-05-4 HCAPLUS
CN 1(2H)-Pyrimidineacetic acid, 3,4-dihydro-5-methyl-2,4-dioxo- (8CI, 9CI) (CA INDEX NAME)



RN 25477-96-7 HCAPLUS
CN 9H-Purine-9-acetic acid, 6-amino-, ethyl ester (8CI, 9CI) (CA INDEX NAME)

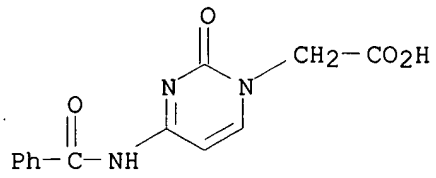


RN 26661-13-2 HCAPLUS
CN Benzamide, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (8CI, 9CI) (CA INDEX NAME)

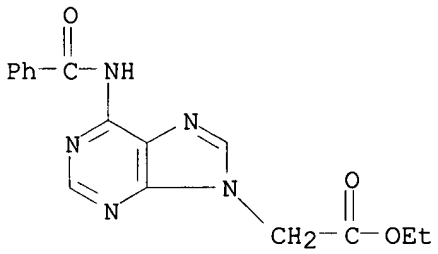


RN 168263-86-3 HCAPLUS
CN 1(2H)-Pyrimidineacetic acid, 4-(benzoylamino)-2-oxo- (9CI) (CA INDEX NAME)

Searched by John Dantzman 308-4488



RN 171406-46-5 HCAPLUS
CN 9H-Purine-9-acetic acid, 6-(benzoylamino)-, ethyl ester (9CI) (CA INDEX NAME)

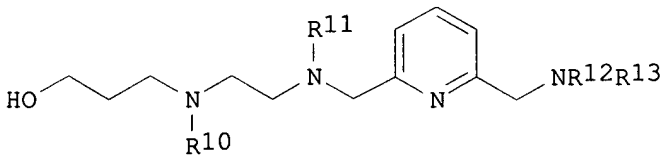


=> d bib abs hitstr l10 3

L10 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:112497 HCAPLUS
DN 128:180338
TI Preparation of compounds or **combinatorial** libraries of compounds having a plurality of nitrogenous substituents
IN **Cook, P. Dan**; An, Haoyun
PA ISIS Pharmaceuticals, Inc., USA; Cook, P. Dan; An, Haoyun
SO PCT Int. Appl., 187 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9805961	A1	19980212	WO 1997-US13530	19970801
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9739036	A1	19980225	AU 1997-39036	19970801
PRAI	US 1996-691206		19960801		
	WO 1997-US13530		19970801		

OS MARPAT 128:180338
GI



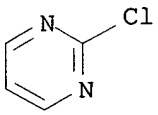
I

AB Novel compds. of general formula L-T-[-N(T-L)(CH2)x-]r-A[(J)t-T-L]-[-(CH2)x-N(T-L)]s-T-L [r = 1-4; s = 2-4; A = arom., **heterocyclic**, alicyclic ring; x = 1-8; J = N, O, S, **heterocyclic** ring system having at least one N; t = 0,1; T = single bond, CH2, [(CR1R2)m-R5-(CR1CR2)n-[C(:R6)]p-E]q; R1, R2 = H, C1-10 alkyl or haloalkyl, C2-10 alkenyl or alkynyl, C6-14 aryl; R5, E = single bond, CH:CH, C.tplbond.C, O, S, (un)substituted NH, SO2, (un)substituted C6-14 aryl, (un)substituted heteroaryl, (un)substituted (mixed) **heterocycle** contg. a N, O, or S; R6 = O, S, (un)substituted NH; m, n = 0-5; p = 0,1; q = 1-10; L = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, or C4-7 carbocyclic alkyl, (un)substituted alkyl, alkenyl, or alkynyl carbocyclic, (un)substituted C6-14 aryl or heteroaryl, (un)substituted **heterocycle** contg. a

N, O, or S, (un)substituted (mixed) **heterocycle**; with proviso that when A = 2,6-disubstituted pyridine with r = s = 2 and 6 of said L groups, then not more than 3 of said L groups are H or p-toluenesulfonyl] are constructed to include a central arom., aliph., or **heterocyclic** ring system. Attached to the central ring system are two linear groups having nitrogenous moieties that are derivatized with chem. functional groups. The ring system can include further nitrogenous moieties, either as ring atoms or on pendant groups attached to the ring, that may also be derivatized with chem. functional groups. The totality of the chem. functional groups imparts certain conformational and other properties to these compds. In accordance with certain embodiments of the invention, libraries of such compds. are prepd. utilizing permutations and **combinations** of the chem. functional groups and the nitrogenous moieties to build complexity into the libraries. Such libraries are useful as antibacterial, antifungal, and imaging agents or for identifying metal chelating species for heavy metal therapy as well as industrial application. Thus, 2-(acetamidomethyl)pyridine deriv. (I; R10 = Boc, R11 = R12 = H, R13 = CH2CONH2) (prepn. given) was alkylated by 3-(trifluoromethyl)benzyl bromide in the presence of K2CO3 in MeCN followed by treatment with CF3CO2H in CHCl3 at room temp. for 4 h to give I (R10 = H, R11 = R12 = 3-(trifluoromethyl)benzyl, R13 = CH2CONH2), which in vitro at 100 .mu.M inhibited 95% Staphylococcus pyogenes and 87% Escherichia coli. Many libraries of compds. were also prepd., e.g., by alkylating I (R10 = Boc, R11 = R12 = R13 = H) with a mixt. of benzyl bromide, 3-fluorobenzyl bromide, .alpha.-bromo-m-xylene, Me 3-bromomethylbenzoate, 3-nitrobenzyl bromide, and 3-(trifluoromethyl)benzyl bromide in MeCN at room temp. overnight followed by deprotection with CF3CO2H to give a library of compds. N-benzylated (hydroxydiazaoctyl)(aminomethyl)pyridine I [R10 = H; R11, R12, R13 are randomly selected from benzyl, 3-fluorobenzyl, 3-methylbenzyl, 3-(methoxycarbonyl)benzyl, 3-nitrobenzyl] having m/z 663-867 in mass spectroscopy, which showed min. inhibitory concn. of 1-5, 1-5, 1-5, and 5-25 .mu.g/mL against Staphylococcus aureus, Staphylococcus pyogenes, Escherichia coli, and Candida albicans, resp., and inhibited 68% phospholipase A2 and 31% tat/TAR RNA/protein interactions at 100 .mu.M, and.

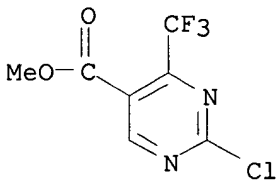
IT **1722-12-9**, 2-Chloropyrimidine **175137-27-6**
RL: RCT (Reactant)
(prepn. of compds. or **combinatorial** libraries of compds. having plurality of nitrogenous substituents as drugs such as antibacterial and antifungal agents)

RN 1722-12-9 HCAPLUS
CN Pyrimidine, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 175137-27-6 HCAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-chloro-4-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

Searched by John Dantzman 308-4488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AN 1995:994352 HCAPLUS
DN 124:146747
TI Preparation of novel phosphoramidate and phophorothioamidate oligomeric compounds
IN **Cook, Phillip Dan**; Acevedo, Oscar; Hebert, Normand
PA Isis Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9523160	A1	19950831	WO 1995-US2267	19950223
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	AU 677150	B2	19970410		
	EP 751948	A1	19970108	EP 1995-912595	19950223
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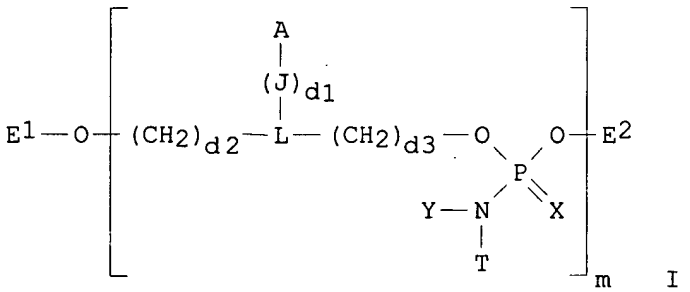

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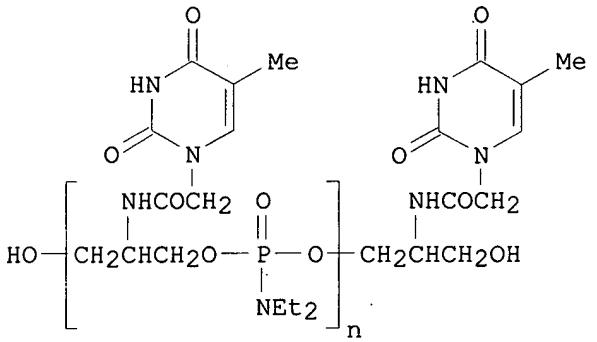


II

AB The title compds.[I; L = backbone segments; Y, T, A = functional groups for (non)interacting with target mols. of interest such as a N-contg. **heterocycle**, purine, pyrimidine, phosphate, polyether, and polyethylene glycol; X = O, S; E1, E2 = H, conjugate groups or intermediate groups used during the synthesis of the compds.; J = linking group such as C1-20 alkyl, CO, C(S), CO2, and CONH; d1 = 0,1; d2 = 0-6; d3 = 1-6; m = 2-50], useful as inhibitors of phospholipase A2, are prepd. using H phosphonate type chem. wherein the functional groups are added during an oxidn. step or during a coupling step. Thus, a thymine-contg. oligomer (II) was prepd. by repeating the steps involving coupling of 1-O-(4,4'-dimethoxytrityl)-N-(9-fluorenylmethoxycarbonyl)-3-amino-1,3-propanediol 3-O-phosphonate to 1-O-(4,4'-dimethoxytrityl)-N-(1-thymin-1-ylacetyl)-2-amino-1,3-propanediol 3-succinate-bound long chain-alkylamino control pore glass support, oxidn. of the resulting H phosphonate with Et2NH to the phosphoramidate, removing the Fmoc-protective group, and reacting the free amine with 1-carboxymethylthymine. Oligomer libraries were also prepd. (only general prepn. given) and screened for inhibition of phospholipase A2 using Escherichia coli labeled with 3H-oleic acid to show specific inhibition for human type II phospholipase A2 (no details for biol. data given).

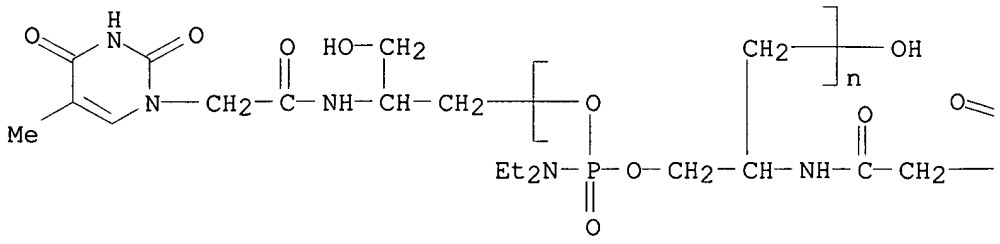
IT **172525-81-4P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel phosphoramidate and phophorothioamidate oligomeric compds. and **combinatorial** libraries as phospholipase A2 inhibitors)

RN 172525-81-4 HCAPLUS

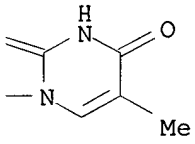
Searched by John Dantzman 308-4488

CN Poly[oxy[(diethylamino)phosphinylidene]oxy[2-[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]-1,3-propanediyl]], .alpha.-[2-[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]-3-hydroxypropyl]-.omega.-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A

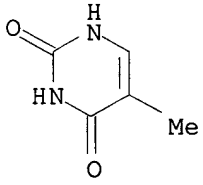


PAGE 1-B

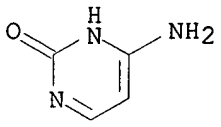


IT **65-71-4**, Thymine **71-30-7**, Cytosine **10310-21-1**, 2-Amino-6-chloropurine **20924-05-4**, 1-Carboxymethylthymine
RL: RCT (Reactant)
(prepn. of novel phosphoramidate and phophorothioamidate oligomeric compds. and **combinatorial** libraries as phospholipase A2 inhibitors)

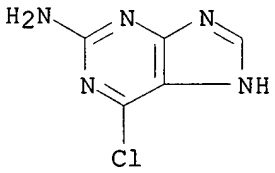
RN 65-71-4 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-methyl- (9CI) (CA INDEX NAME)



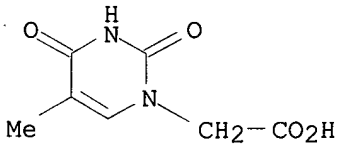
RN 71-30-7 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino- (9CI) (CA INDEX NAME)



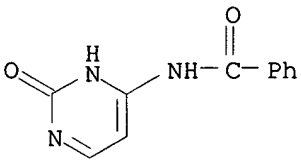
RN 10310-21-1 HCAPLUS
CN 1H-Purin-2-amine, 6-chloro- (9CI) (CA INDEX NAME)



RN 20924-05-4 HCAPLUS
CN 1(2H)-Pyrimidineacetic acid, 3,4-dihydro-5-methyl-2,4-dioxo- (8CI, 9CI) (CA INDEX NAME)

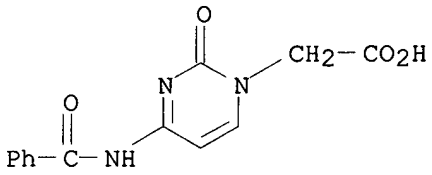


IT **26661-13-2P**, N4-Benzoylcytosine **168263-86-3P**, N4-Benzoyl-1-cytosinylacetic acid **171406-46-5P**, Ethyl 9-adenylacetate **171486-04-7P**, N6-Benzoyl-9-adenylacetic acid **172405-20-8P**, N2-Isobutyryl-9-guanylacetic acid **172525-49-4DP**, long chain alkylamine control pore glass-bound **172525-55-2DP**, long chain alkylamine control pore glass-bound **172525-56-3DP**, long chain alkylamine control pore glass-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of novel phosphoramidate and phophorothioamidate oligomeric compds. and **combinatorial** libraries as phospholipase A2 inhibitors)
RN 26661-13-2 HCAPLUS
CN Benzamide, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (8CI, 9CI) (CA INDEX NAME)

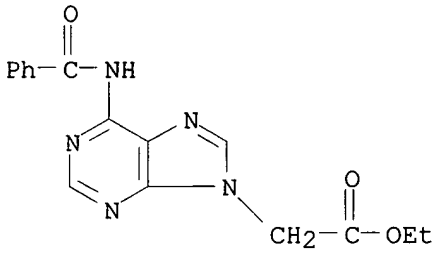


RN 168263-86-3 HCAPLUS

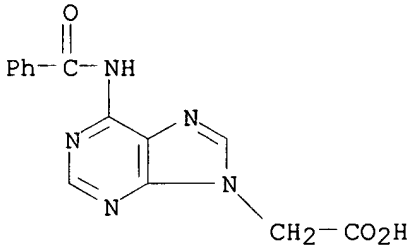
CN 1(2H)-Pyrimidineacetic acid, 4-(benzoylamino)-2-oxo- (9CI) (CA INDEX NAME)



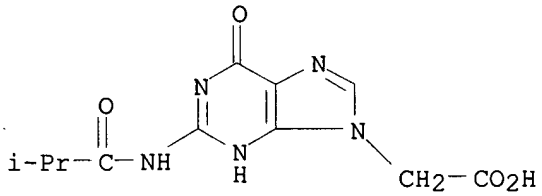
RN 171406-46-5 HCAPLUS
CN 9H-Purine-9-acetic acid, 6-(benzoylamino)-, ethyl ester (9CI) (CA INDEX NAME)



RN 171486-04-7 HCAPLUS
CN 9H-Purine-9-acetic acid, 6-(benzoylamino)- (9CI) (CA INDEX NAME)

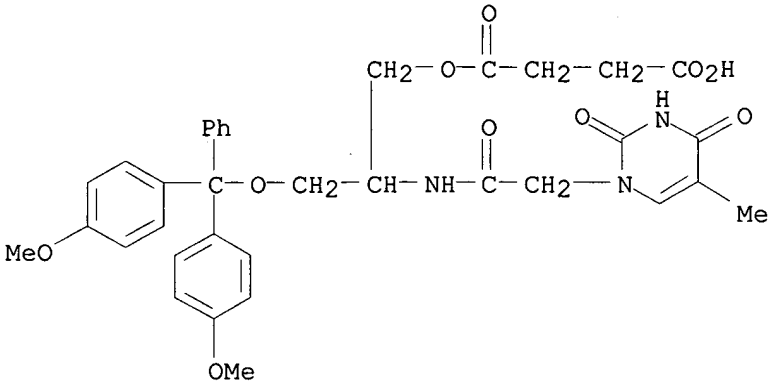


RN 172405-20-8 HCAPLUS
CN 9H-Purine-9-acetic acid, 1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo- (9CI) (CA INDEX NAME)

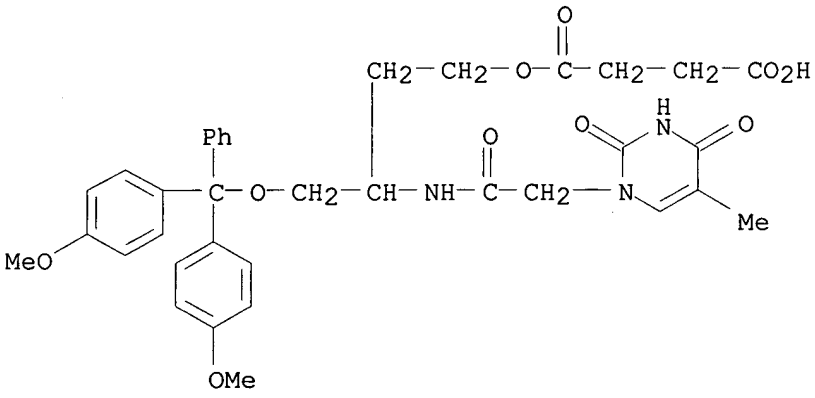


Searched by John Dantzman 308-4488

RN 172525-49-4 HCAPLUS
CN Butanedioic acid, mono[3-[bis(4-methoxyphenyl)phenylmethoxy]-2-[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]propyl] ester (9CI) (CA INDEX NAME)



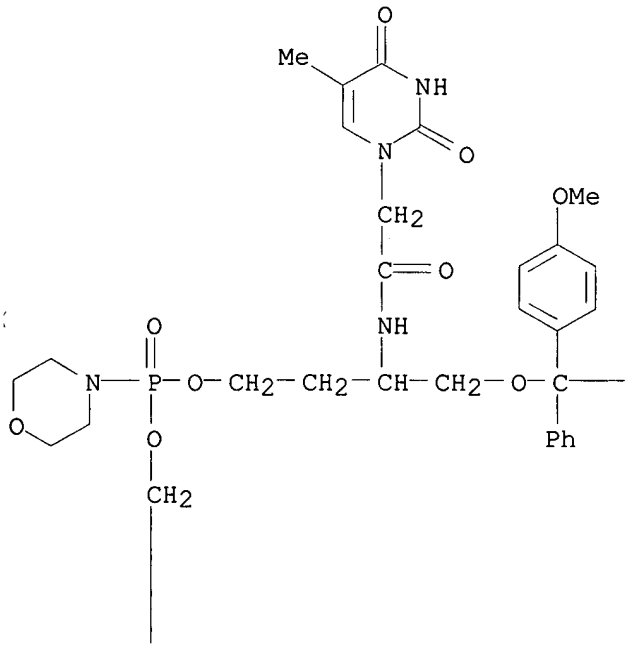
RN 172525-55-2 HCAPLUS
CN Butanedioic acid, mono[4-[bis(4-methoxyphenyl)phenylmethoxy]-3-[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]butyl] ester (9CI) (CA INDEX NAME)



RN 172525-56-3 HCAPLUS
CN Butanedioic acid,
mono[3,10,17-tris[[(3,4-dihydro-5-methyl-2,5-dioxo-1(2H)-

pyrimidinyl)acetyl]amino]-20,20-bis(4-methoxyphenyl)-6,13-di-4-morpholinyl-6,13-dioxido-20-phenyl-5,7,12,14,19-pentaoxa-6,13-diphosphaeicos-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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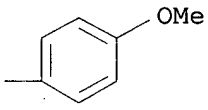

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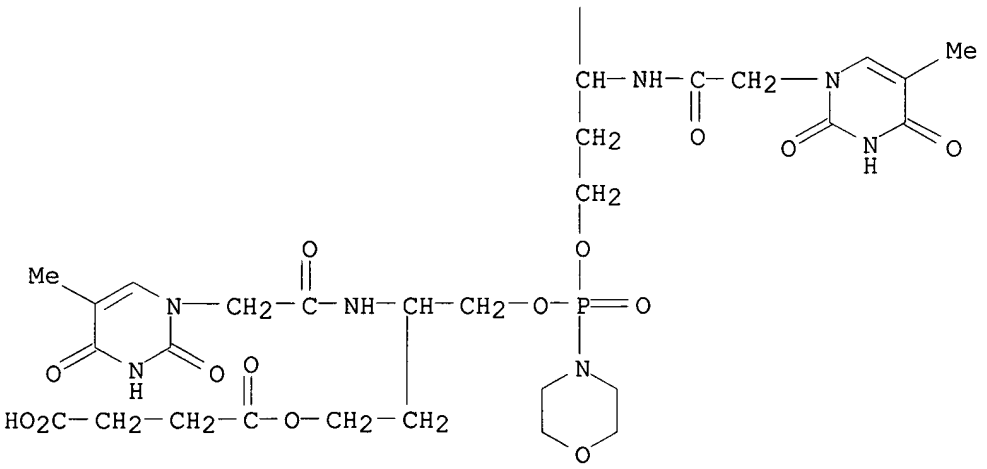
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